# Glutaric acid, hex-4-yn-3-yl 4-biphenyl ester

**Inchi:** InChI=1S/C23H24O4/c1-3-9-20(4-2)26-22(24)12-8-13-23(25)27-21-16-14-19(15-17-21)1
**InchiKey:** XFZLKYYXIBENKO-UHFFFAOYSA-N
**Formula:** C23H24O4
**SMILES:** CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(-c2ccccc2)cc1
**Mol. weight [g/mol]:** 364.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 90.49 | kJ/mol | Joback Method |
| hf | -279.04 | kJ/mol | Joback Method |
| hfus | 48.19 | kJ/mol | Joback Method |
| hvap | 92.08 | kJ/mol | Joback Method |
| log10ws | -6.92 | | Crippen Method |
| logp | 4.774 | | Crippen Method |
| mcvol | 293.690 | ml/mol | McGowan Method |
| pc | 1575.95 | kPa | Joback Method |
| rinpol | 2898.00 | | NIST Webbook |
| rinpol | 2898.00 | | NIST Webbook |
| tb | 945.12 | K | Joback Method |
| tc | 1182.31 | K | Joback Method |
| tf | 649.75 | K | Joback Method |
| vc | 1.111 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 901.62 | J/mol×K | 945.12 | Joback Method |
| cpg | 915.35 | J/mol×K | 984.65 | Joback Method |
| cpg | 927.63 | J/mol×K | 1024.18 | Joback Method |
| cpg | 938.51 | J/mol×K | 1063.72 | Joback Method |
| cpg | 948.06 | J/mol×K | 1103.25 | Joback Method |
| cpg | 956.31 | J/mol×K | 1142.78 | Joback Method |
| cpg | 963.32 | J/mol×K | 1182.31 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390124&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |